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Diaquatetrakis(1,3-di-4-pyridylpropane-κN)manganese(II) bis(hexafluoridophosphate) monohydrate

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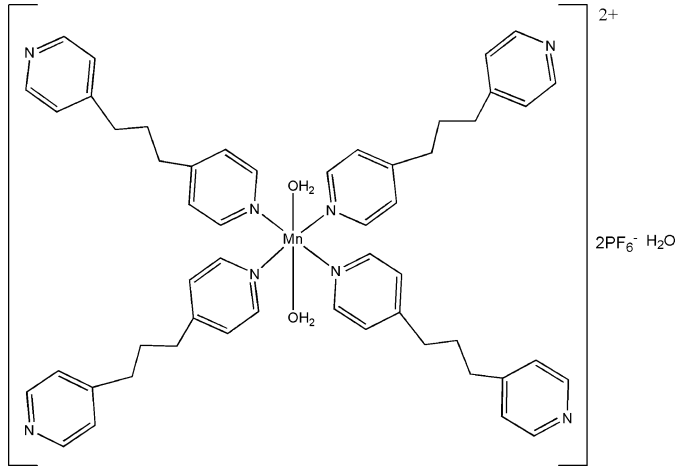
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.046; wR factor = 0.135; data-to-parameter ratio = 12.9.

The title mononuclear Mn^{II} complex, $[Mn(C_{13}H_{14}N_2)_4(H_2O)_2](PF_6)_2\cdot H_2O$, is isostructural with the previously reported Zn^{II} complex. The metal center is coordinated by four monodentate 1,3-di-4-pyridylpropane ($L1$) ligands and two water molecules. One $L1$ ligand is affected by disorder of two propane C atoms, which are distributed over two positions, with occupancies 0.771 (8)/0.229 (8). The asymmetric unit is completed by one solvent water molecule and two PF_6^- anions, both disordered over two positions, with occupancies for F atoms of 0.621 (10)/0.379 (10) for one anion and 0.69 (2)/0.31 (2) for the other. Uncoordinated N atoms of pyridyl groups belonging to $L1$ and water molecules are involved in hydrogen bonds, with $D\cdots A$ separations ranging from 1.85 (4) to 2.07 (4) Å and D—H$\cdots A$ angles from 169 (3) to 174 (4)°.

Related literature

For related structures based on the ligand $L1$, see: Belcher *et al.* (2002); Bujaci *et al.* (2002); Carlucci *et al.* (2002); Hu & Tong (2005); Plater *et al.* (2000). A Zn^{II} complex isostructural with the title complex has been crystallographically characterized by Kim *et al.* (2006). The same Zn^{II}-based cation has also been crystallized using ClO_4^- as anions (Choi *et al.*, 2004).



Experimental

Crystal data

$[Mn(C_{13}H_{14}N_2)_4(H_2O)_2](PF_6)_2\cdot H_2O$
M_r = 1191.98
Orthorhombic, *Pbca*
a = 19.1098 (15) Å
b = 16.1767 (13) Å
c = 38.158 (3) Å
V = 11795.9 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 291 (2) K
0.47 × 0.38 × 0.37 mm

Data collection

Bruker SMART APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.848, T_{max} = 0.878
85755 measured reflections
10983 independent reflections
7230 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
S = 1.02
10983 reflections
850 parameters
30 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O2—H21$\cdots$O1	0.85 (4)	1.85 (4)	2.693 (3)	173 (3)
O1—H11$\cdots$N7^{i}	0.85 (4)	1.94 (4)	2.775 (3)	169 (3)
O1—H12$\cdots$N8^{ii}	0.86 (4)	1.90 (4)	2.752 (3)	172 (3)
O2—H22$\cdots$N5^{iii}	0.80 (4)	2.02 (4)	2.818 (3)	174 (4)
O3—H31$\cdots$N6^{iv}	0.79 (4)	2.07 (4)	2.861 (3)	174 (4)
O3—H32$\cdots$O1^{v}	0.83 (4)	1.92 (4)	2.733 (3)	169 (3)

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x+\frac{3}{2}, y-\frac{1}{2}, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2123).

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supplementary materials

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Diaquatetrakis(1,3-di-4-pyridylpropane-*κN*)manganese(II) bis(hexafluoridophosphate) monohydrate

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Comment

The ligand 1,3-bis(4-pyridyl)propane (*L*1) has been usually used as a nitrogen donor bridging ligand (Belcher *et al.*, 2002; Plater *et al.*, 2000; Bujaci *et al.*, 2002; Hu & Tong, 2005; Carlucci *et al.*, 2002). However, when *L*1 and *L*2 [2,5-bis(2-pyridyl)-1,3,4-thiadiazole, which is usually used as an angular bridging ligand] coexisted in a self-assembling system with $Mn(CH_3COO)_2$ and NH_4PF_6, the title mononuclear manganese(II) complex, (I), was formed, where *L*1 is coordinated to Mn^{II} in a monodentate mode. Two Zn^{II} mononuclear complexes including *L*1 have reported (Choi *et al.*, 2004; Kim *et al.*, 2006). Both have structures very similar to that of (I).

In (I), the metal centre Mn^{II} coordinates to four N atoms from four crystallographically independent bridging ligands *L*1, and two O atoms from two distinct water molecules, to form an octahedral coordination geometry. The Mn—N distances fall in the range 2.267 (2)–2.286 (2) Å and the Mn—O distances in the range 2.1829 (19)–2.196 (2) Å. The angles N—Mn—O vary from 84.69 (8) to 94.28 (8)° (Fig. 1). Furthermore, the major contributors to the construction of supramolecular systems are hydrogen bonds between N atoms of non-coordinated pyridyl rings and O atoms of water molecules, and between O atom of the lattice water molecule and O atoms of coordinating water molecules. The H···Acceptor separations for these contacts vary from 1.85 (4) to 2.07 (4) Å, while *D*—H···*A* angles are close to 175°, indicating that these hydrogen bonds may be considered as strong interactions.

Experimental

To a solution of *L*1 (0.02 g, 0.1 mmol) and *L*2 (0.024 g, 0.1 mmol) in a mixture of solvents (5 ml chloroform, 10 ml me thanol) was added a solution of $Mn(CH_3COO)_2$ (0.025 g, 0.1 mmol) in methanol (10 ml). NH_4PF_6 (0.033 g, 0.2 mmol) in water (5 ml) was added to the mixture after it was stirred for 20 min. After being stirred for another 5 min., the mixture was filtered. The filtrate was allowed to slowly evaporate at room temperature and after *ca*. 20 days, suitable single crystals (yellow block) were obtained. Yield: 65%.

Refinement

Atoms C20 and C21 belonging to the propane chain of a *L*1 ligand are disordered over two positions and their occupancies converged to 0.771 (8) [C20/C21] and 0.229 (8) [C20'/C21']. Corresponding C—C bond lengths were restrained to 1.54 (1) Å. Two PF_6^- anions are also disordered, each F atom being found over two positions. Site occupation factors for each group of six F atoms converged to 0.621 (10)/0.379 (10) [P1 anion] and 0.69 (2)/0.31 (2) [P2 anion]. P—F bond lengths were restrained to 1.56 (1) Å. C-bounded H atoms were placed at calculated positions (C—H = 0.93 Å for pyridyl rings, C—H = 0.97 Å for methylene groups), and they were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(carrier C). Water H atoms were found in a difference map and refined freely, with U_{iso}(H) = 1.5U_{eq}(carrier O).

Figures

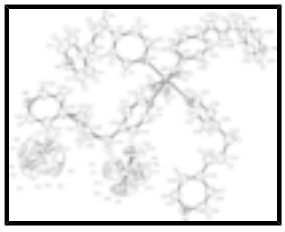

Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

Diaquatetrakis(1,3-di-4-pyridylpropane-κ*N*)manganese(II) bis(hexafluoridophosphate) monohydrate

Crystal data

$[Mn(C_{13}H_{14}N_2)_4(H_2O)_2](PF_6)_2·H_2O$	F_{000} = 4936
M_r = 1191.98	D_x = 1.342 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	θ = 2.3–25.5º
a = 19.1098 (15) Å	μ = 0.36 mm^{-1}
b = 16.1767 (13) Å	*T* = 291 (2) K
c = 38.158 (3) Å	Block, yellow
V = 11795.9 (16) Å^3	0.47 × 0.38 × 0.37 mm
Z = 8	

Data collection

Bruker SMART APEXII diffractometer	10983 independent reflections
Radiation source: fine-focus sealed tube	7230 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.052
T = 291(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2001)	*h* = −23→23
T_{min} = 0.848, T_{max} = 0.878	*k* = −19→19
85755 measured reflections	*l* = −45→46

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.135	$w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 6.7503P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001

10983 reflections	$\Delta\rho_{max}$ = 0.59 e Å^{-3}
850 parameters	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
30 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mn1	0.70400 (2)	0.02454 (2)	0.133707 (10)	0.04321 (12)	
N1	0.70839 (12)	0.02343 (13)	0.19354 (6)	0.0480 (5)	
N2	0.58464 (11)	0.02697 (13)	0.13621 (6)	0.0489 (5)	
N3	0.69837 (12)	0.01830 (14)	0.07391 (6)	0.0504 (6)	
N4	0.82242 (12)	0.02855 (14)	0.13048 (6)	0.0506 (6)	
N5	0.38951 (13)	−0.23584 (16)	0.32703 (7)	0.0629 (7)	
N6	0.35463 (13)	0.29250 (15)	0.30557 (6)	0.0574 (6)	
N7	0.40863 (14)	0.24093 (17)	−0.07644 (7)	0.0663 (7)	
N8	1.19755 (15)	0.19365 (19)	−0.03144 (7)	0.0736 (8)	
O2	0.70152 (11)	0.15938 (12)	0.13552 (6)	0.0551 (5)	
H21	0.7248 (18)	0.190 (2)	0.1216 (9)	0.083*	
H22	0.6778 (19)	0.189 (2)	0.1474 (9)	0.083*	
O3	0.70263 (11)	−0.11068 (12)	0.13860 (5)	0.0536 (5)	
H31	0.6838 (19)	−0.136 (2)	0.1537 (9)	0.080*	
H32	0.7156 (18)	−0.144 (2)	0.1234 (9)	0.080*	
C1	0.66266 (15)	0.06664 (17)	0.21287 (7)	0.0523 (7)	
H1A	0.6353	0.1063	0.2018	0.063*	
C2	0.65415 (15)	0.05526 (17)	0.24825 (7)	0.0538 (7)	
H2A	0.6218	0.0871	0.2604	0.065*	
C3	0.69330 (15)	−0.00320 (18)	0.26594 (7)	0.0500 (7)	
C4	0.74253 (15)	−0.04584 (18)	0.24613 (7)	0.0554 (7)	
H4A	0.7716	−0.0845	0.2568	0.066*	
C5	0.74827 (15)	−0.03088 (18)	0.21080 (7)	0.0532 (7)	
H5A	0.7818	−0.0602	0.1982	0.064*	
C6	0.68197 (17)	−0.0221 (2)	0.30402 (7)	0.0637 (8)	
H6A	0.6674	0.0280	0.3160	0.076*	
H6B	0.7259	−0.0398	0.3143	0.076*	
C7	0.62675 (16)	−0.0893 (2)	0.30997 (8)	0.0686 (9)	
H7A	0.6407	−0.1386	0.2973	0.082*	
H7B	0.6258	−0.1031	0.3347	0.082*	
C8	0.55431 (17)	−0.0657 (2)	0.29867 (8)	0.0671 (9)	
H8A	0.5543	−0.0585	0.2734	0.080*	
H8B	0.5428	−0.0127	0.3091	0.080*	
C9	0.49752 (16)	−0.12680 (19)	0.30818 (8)	0.0587 (8)	
C10	0.49169 (19)	−0.1582 (2)	0.34163 (8)	0.0734 (10)	
H10A	0.5243	−0.1438	0.3587	0.088*	
C11	0.43765 (19)	−0.2109 (2)	0.34977 (9)	0.0714 (9)	
H11A	0.4346	−0.2303	0.3727	0.086*	
C12	0.39608 (16)	−0.2064 (2)	0.29469 (9)	0.0703 (9)	

H12A	0.3636	−0.2230	0.2779	0.084*
C13	0.44810 (16)	−0.1528 (2)	0.28455 (8)	0.0672 (9)
H13A	0.4498	−0.1340	0.2615	0.081*
C14	0.54721 (16)	0.08366 (19)	0.11880 (8)	0.0579 (7)
H14A	0.5697	0.1149	0.1017	0.069*
C15	0.47712 (16)	0.0981 (2)	0.12486 (9)	0.0643 (8)
H15A	0.4535	0.1381	0.1120	0.077*
C16	0.44203 (15)	0.05300 (19)	0.15018 (8)	0.0571 (8)
C17	0.47996 (16)	−0.00749 (19)	0.16718 (9)	0.0610 (8)
H17A	0.4582	−0.0411	0.1837	0.073*
C18	0.54969 (15)	−0.01827 (17)	0.15976 (8)	0.0561 (7)
H18A	0.5739	−0.0593	0.1718	0.067*
C22	0.37837 (16)	0.1846 (2)	0.24928 (9)	0.0729 (10)
C23	0.31141 (16)	0.2026 (2)	0.26098 (9)	0.0694 (9)
H23A	0.2727	0.1792	0.2501	0.083*
C24	0.30269 (15)	0.2554 (2)	0.28881 (8)	0.0595 (8)
H24A	0.2573	0.2658	0.2964	0.071*
C25	0.41872 (16)	0.2757 (2)	0.29401 (8)	0.0628 (8)
H25A	0.4564	0.3009	0.3052	0.075*
C26	0.43244 (16)	0.2234 (2)	0.26657 (9)	0.0693 (9)
H26A	0.4784	0.2141	0.2596	0.083*
C27	0.65185 (17)	−0.03113 (19)	0.05824 (8)	0.0620 (8)
H27A	0.6230	−0.0635	0.0723	0.074*
C28	0.64433 (19)	−0.0368 (2)	0.02254 (8)	0.0694 (9)
H28A	0.6107	−0.0719	0.0131	0.083*
C29	0.68607 (18)	0.0092 (2)	0.00059 (8)	0.0614 (8)
C30	0.73450 (18)	0.0595 (2)	0.01643 (8)	0.0655 (9)
H30A	0.7644	0.0915	0.0028	0.079*
C31	0.73895 (17)	0.06293 (19)	0.05251 (8)	0.0614 (8)
H31A	0.7719	0.0981	0.0625	0.074*
C32	0.6772 (2)	0.0041 (2)	−0.03861 (8)	0.0840 (11)
H32A	0.6775	−0.0534	−0.0457	0.101*
H32B	0.7165	0.0313	−0.0499	0.101*
C33	0.6092 (2)	0.0444 (2)	−0.05118 (9)	0.0806 (11)
H33A	0.6025	0.0313	−0.0758	0.097*
H33B	0.5703	0.0207	−0.0383	0.097*
C34	0.60789 (18)	0.1369 (2)	−0.04674 (9)	0.0730 (9)
H34A	0.6177	0.1504	−0.0225	0.088*
H34B	0.6445	0.1612	−0.0610	0.088*
C35	0.53863 (16)	0.17413 (19)	−0.05695 (8)	0.0592 (8)
C36	0.49404 (17)	0.2096 (2)	−0.03281 (8)	0.0659 (8)
H36A	0.5067	0.2116	−0.0093	0.079*
C37	0.43133 (18)	0.2420 (2)	−0.04330 (9)	0.0710 (9)
H37A	0.4028	0.2661	−0.0264	0.085*
C38	0.51575 (17)	0.1736 (2)	−0.09127 (8)	0.0659 (8)
H38A	0.5436	0.1505	−0.1087	0.079*
C39	0.45195 (18)	0.2071 (2)	−0.09974 (8)	0.0656 (8)
H39A	0.4381	0.2061	−0.1231	0.079*
C40	0.85845 (15)	−0.01861 (19)	0.10818 (8)	0.0621 (8)

H40A	0.8346	−0.0595	0.0959	0.074*	
C41	0.92900 (15)	−0.0097 (2)	0.10251 (9)	0.0654 (9)	
H41A	0.9515	−0.0437	0.0864	0.078*	
C42	0.96675 (14)	0.04918 (17)	0.12054 (7)	0.0502 (7)	
C43	0.92954 (15)	0.09603 (18)	0.14435 (8)	0.0550 (7)	
H43A	0.9525	0.1356	0.1578	0.066*	
C44	0.85903 (15)	0.08460 (18)	0.14835 (8)	0.0564 (7)	
H44A	0.8354	0.1177	0.1644	0.068*	
C45	1.04368 (15)	0.0626 (2)	0.11425 (8)	0.0610 (8)	
H45A	1.0687	0.0116	0.1190	0.073*	
H45B	1.0608	0.1043	0.1304	0.073*	
C46	1.05902 (15)	0.0898 (2)	0.07694 (8)	0.0633 (8)	
H46A	1.0422	0.0479	0.0608	0.076*	
H46B	1.0337	0.1405	0.0721	0.076*	
C47	1.13549 (17)	0.1040 (3)	0.07062 (9)	0.0812 (11)	
H47A	1.1599	0.0522	0.0745	0.097*	
H47B	1.1524	0.1430	0.0880	0.097*	
C48	1.15515 (16)	0.1361 (2)	0.03462 (8)	0.0622 (8)	
C49	1.21620 (16)	0.1777 (2)	0.02998 (9)	0.0637 (8)	
H49A	1.2451	0.1883	0.0491	0.076*	
C50	1.23538 (18)	0.2040 (2)	−0.00279 (10)	0.0729 (9)	
H50A	1.2781	0.2312	−0.0050	0.087*	
C51	1.1365 (2)	0.1568 (3)	−0.02687 (9)	0.0916 (13)	
H51A	1.1072	0.1508	−0.0462	0.110*	
C52	1.11397 (19)	0.1266 (3)	0.00503 (9)	0.0899 (12)	
H52A	1.0710	0.0998	0.0066	0.108*	
C19	0.36677 (15)	0.0712 (2)	0.15932 (9)	0.0786 (11)	
H19A	0.3450	0.0217	0.1687	0.094*	0.771 (8)
H19B	0.3416	0.0870	0.1383	0.094*	0.771 (8)
H19C	0.3390	0.0226	0.1539	0.094*	0.229 (8)
H19D	0.3501	0.1161	0.1447	0.094*	0.229 (8)
C20	0.3620 (3)	0.1425 (4)	0.18699 (12)	0.0720 (18)	0.771 (8)
H20A	0.3881	0.1900	0.1786	0.086*	0.771 (8)
H20B	0.3135	0.1591	0.1897	0.086*	0.771 (8)
C21	0.3905 (2)	0.1160 (3)	0.22211 (11)	0.0676 (15)	0.771 (8)
H21A	0.4402	0.1047	0.2201	0.081*	0.771 (8)
H21B	0.3674	0.0657	0.2297	0.081*	0.771 (8)
C20'	0.3532 (8)	0.0952 (10)	0.1981 (3)	0.058 (5)	0.229 (8)
H20C	0.3033	0.1019	0.2017	0.069*	0.229 (8)
H20D	0.3690	0.0506	0.2131	0.069*	0.229 (8)
C21'	0.3904 (8)	0.1748 (9)	0.2085 (3)	0.068 (5)	0.229 (8)
H21C	0.3709	0.2216	0.1960	0.081*	0.229 (8)
H21D	0.4400	0.1712	0.2033	0.081*	0.229 (8)
O1	0.76697 (12)	0.26568 (13)	0.09221 (5)	0.0539 (5)	
H11	0.8099 (19)	0.257 (2)	0.0877 (9)	0.081*	
H12	0.7416 (18)	0.276 (2)	0.0741 (9)	0.081*	
P1	0.35340 (5)	0.77112 (6)	0.18112 (3)	0.0767 (3)	
F1	0.3712 (9)	0.7158 (5)	0.2114 (3)	0.245 (7)	0.621 (10)
F2	0.4294 (2)	0.7681 (6)	0.1668 (2)	0.136 (3)	0.621 (10)

F3	0.3396 (4)	0.8378 (4)	0.15195 (19)	0.142 (3)	0.621 (10)
F4	0.2810 (4)	0.7827 (6)	0.1969 (3)	0.196 (5)	0.621 (10)
F5	0.3286 (7)	0.7040 (7)	0.1565 (3)	0.166 (5)	0.621 (10)
F6	0.3765 (5)	0.8453 (5)	0.20553 (16)	0.137 (3)	0.621 (10)
F1'	0.3395 (17)	0.7567 (16)	0.2200 (2)	0.261 (12)	0.379 (10)
F2'	0.4146 (6)	0.7104 (9)	0.1898 (6)	0.207 (8)	0.379 (10)
F3'	0.3745 (17)	0.7700 (16)	0.1434 (3)	0.305 (13)	0.379 (10)
F4'	0.2840 (7)	0.8135 (10)	0.1774 (4)	0.204 (9)	0.379 (10)
F5'	0.3208 (14)	0.6859 (9)	0.1761 (6)	0.171 (8)	0.379 (10)
F6'	0.3954 (15)	0.8467 (12)	0.1908 (7)	0.315 (15)	0.379 (10)
P2	0.40249 (6)	0.30718 (7)	0.06184 (2)	0.0810 (3)	
F7	0.3604 (18)	0.266 (2)	0.0919 (7)	0.186 (13)	0.31 (2)
F8	0.3344 (11)	0.3209 (17)	0.0405 (9)	0.168 (12)	0.31 (2)
F9	0.4496 (11)	0.3548 (19)	0.0352 (6)	0.174 (11)	0.31 (2)
F10	0.4715 (8)	0.2748 (10)	0.0803 (6)	0.134 (8)	0.31 (2)
F11	0.414 (2)	0.2321 (11)	0.0380 (5)	0.202 (13)	0.31 (2)
F12	0.383 (2)	0.3841 (13)	0.0838 (7)	0.200 (12)	0.31 (2)
F7'	0.3766 (6)	0.2576 (8)	0.0937 (2)	0.125 (3)	0.69 (2)
F8'	0.3277 (5)	0.3342 (8)	0.0529 (4)	0.155 (4)	0.69 (2)
F9'	0.4278 (9)	0.3532 (7)	0.0284 (3)	0.191 (6)	0.69 (2)
F10'	0.4790 (3)	0.2858 (8)	0.0716 (4)	0.186 (5)	0.69 (2)
F11'	0.3940 (5)	0.2242 (4)	0.0411 (2)	0.122 (3)	0.69 (2)
F12'	0.4130 (7)	0.3878 (4)	0.0841 (2)	0.136 (3)	0.69 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.0426 (2)	0.0421 (2)	0.0450 (2)	0.00177 (18)	0.01101 (17)	0.00263 (18)
N1	0.0525 (13)	0.0439 (12)	0.0476 (12)	0.0015 (11)	0.0086 (11)	−0.0003 (11)
N2	0.0439 (12)	0.0441 (13)	0.0588 (14)	0.0006 (10)	0.0106 (11)	0.0024 (11)
N3	0.0583 (15)	0.0454 (13)	0.0474 (13)	−0.0014 (12)	0.0088 (11)	0.0030 (11)
N4	0.0449 (13)	0.0491 (13)	0.0577 (14)	0.0024 (11)	0.0120 (11)	−0.0037 (12)
N5	0.0594 (16)	0.0610 (16)	0.0683 (17)	−0.0131 (13)	0.0147 (13)	−0.0029 (13)
N6	0.0574 (16)	0.0578 (15)	0.0572 (15)	0.0065 (12)	0.0057 (12)	−0.0033 (12)
N7	0.0591 (16)	0.0758 (18)	0.0641 (17)	−0.0091 (14)	−0.0053 (14)	0.0088 (14)
N8	0.0661 (18)	0.091 (2)	0.0638 (17)	0.0013 (16)	0.0113 (15)	−0.0027 (15)
O2	0.0585 (13)	0.0400 (11)	0.0669 (14)	0.0021 (9)	0.0256 (10)	0.0054 (9)
O3	0.0690 (14)	0.0406 (11)	0.0511 (12)	0.0002 (10)	0.0135 (10)	0.0002 (9)
C1	0.0604 (18)	0.0443 (16)	0.0523 (17)	0.0021 (13)	0.0090 (14)	0.0017 (13)
C2	0.0589 (18)	0.0491 (16)	0.0534 (17)	−0.0044 (14)	0.0144 (14)	−0.0074 (14)
C3	0.0518 (17)	0.0532 (16)	0.0449 (15)	−0.0190 (13)	0.0029 (13)	−0.0036 (13)
C4	0.0541 (17)	0.0589 (18)	0.0532 (17)	−0.0020 (14)	−0.0055 (14)	0.0058 (14)
C5	0.0500 (16)	0.0567 (18)	0.0529 (17)	0.0045 (14)	0.0060 (13)	−0.0017 (14)
C6	0.0648 (19)	0.083 (2)	0.0436 (16)	−0.0239 (17)	−0.0022 (14)	0.0001 (15)
C7	0.066 (2)	0.087 (2)	0.0536 (18)	−0.0141 (18)	0.0038 (15)	0.0158 (17)
C8	0.071 (2)	0.072 (2)	0.0577 (18)	−0.0184 (17)	0.0011 (16)	0.0155 (16)
C9	0.0610 (19)	0.0630 (19)	0.0519 (17)	−0.0137 (15)	0.0029 (14)	0.0056 (14)
C10	0.087 (2)	0.081 (2)	0.0528 (18)	−0.035 (2)	−0.0044 (17)	0.0080 (17)

C11	0.088 (3)	0.071 (2)	0.0554 (19)	−0.0243 (19)	0.0089 (18)	0.0092 (16)
C12	0.0528 (19)	0.091 (3)	0.067 (2)	−0.0154 (17)	0.0021 (16)	−0.0005 (19)
C13	0.0604 (19)	0.087 (2)	0.0539 (18)	−0.0181 (17)	−0.0011 (15)	0.0139 (17)
C14	0.0549 (18)	0.0577 (18)	0.0610 (18)	0.0012 (15)	0.0049 (14)	0.0080 (15)
C15	0.0536 (19)	0.067 (2)	0.072 (2)	0.0103 (16)	−0.0086 (16)	−0.0051 (17)
C16	0.0420 (16)	0.0633 (19)	0.0662 (19)	−0.0035 (14)	0.0026 (14)	−0.0270 (16)
C17	0.0556 (19)	0.0523 (18)	0.075 (2)	−0.0111 (15)	0.0205 (16)	−0.0083 (16)
C18	0.0519 (17)	0.0450 (16)	0.0714 (19)	0.0004 (14)	0.0144 (15)	0.0040 (14)
C22	0.0505 (18)	0.093 (3)	0.075 (2)	0.0004 (18)	0.0081 (16)	−0.0315 (19)
C23	0.0454 (18)	0.085 (2)	0.078 (2)	−0.0009 (16)	0.0049 (15)	−0.0235 (19)
C24	0.0444 (17)	0.069 (2)	0.0658 (19)	0.0068 (15)	0.0134 (15)	−0.0023 (16)
C25	0.0529 (19)	0.068 (2)	0.067 (2)	−0.0042 (15)	0.0006 (15)	−0.0077 (16)
C26	0.0459 (18)	0.086 (2)	0.076 (2)	−0.0011 (16)	0.0127 (16)	−0.0210 (19)
C27	0.067 (2)	0.0555 (18)	0.0635 (19)	−0.0110 (16)	0.0054 (16)	0.0075 (15)
C28	0.083 (2)	0.064 (2)	0.061 (2)	−0.0053 (18)	−0.0125 (17)	−0.0039 (16)
C29	0.077 (2)	0.0566 (18)	0.0502 (17)	0.0181 (17)	0.0019 (16)	0.0008 (14)
C30	0.080 (2)	0.065 (2)	0.0514 (18)	0.0003 (18)	0.0166 (16)	0.0113 (16)
C31	0.068 (2)	0.0598 (19)	0.0558 (18)	−0.0119 (16)	0.0109 (15)	0.0032 (15)
C32	0.114 (3)	0.084 (2)	0.055 (2)	0.032 (2)	−0.006 (2)	−0.0059 (18)
C33	0.110 (3)	0.068 (2)	0.063 (2)	0.008 (2)	−0.019 (2)	−0.0084 (17)
C34	0.072 (2)	0.068 (2)	0.079 (2)	−0.0027 (18)	−0.0117 (18)	−0.0036 (18)
C35	0.0628 (19)	0.0544 (18)	0.0604 (19)	−0.0077 (15)	−0.0041 (15)	0.0021 (15)
C36	0.067 (2)	0.078 (2)	0.0520 (18)	−0.0078 (17)	−0.0096 (16)	0.0012 (16)
C37	0.067 (2)	0.088 (2)	0.059 (2)	−0.0044 (19)	0.0020 (17)	−0.0039 (18)
C38	0.071 (2)	0.074 (2)	0.0533 (18)	−0.0004 (17)	0.0023 (16)	−0.0016 (16)
C39	0.072 (2)	0.074 (2)	0.0508 (18)	−0.0120 (18)	−0.0068 (16)	0.0083 (16)
C40	0.0473 (17)	0.0565 (18)	0.082 (2)	−0.0019 (14)	0.0132 (15)	−0.0248 (16)
C41	0.0493 (18)	0.067 (2)	0.079 (2)	0.0020 (15)	0.0172 (16)	−0.0292 (17)
C42	0.0462 (16)	0.0533 (16)	0.0512 (16)	0.0007 (13)	0.0085 (13)	0.0006 (13)
C43	0.0526 (18)	0.0539 (17)	0.0586 (17)	−0.0032 (14)	0.0075 (14)	−0.0104 (14)
C44	0.0540 (18)	0.0569 (18)	0.0583 (17)	0.0033 (14)	0.0130 (14)	−0.0152 (15)
C45	0.0461 (17)	0.072 (2)	0.0648 (19)	−0.0044 (15)	0.0103 (14)	−0.0062 (16)
C46	0.0468 (17)	0.0631 (19)	0.080 (2)	0.0026 (15)	0.0164 (15)	0.0073 (16)
C47	0.056 (2)	0.115 (3)	0.073 (2)	−0.012 (2)	0.0145 (17)	0.003 (2)
C48	0.0484 (17)	0.073 (2)	0.065 (2)	−0.0003 (15)	0.0141 (15)	−0.0080 (16)
C49	0.0499 (18)	0.071 (2)	0.070 (2)	−0.0004 (16)	0.0001 (15)	0.0039 (17)
C50	0.060 (2)	0.079 (2)	0.080 (2)	−0.0052 (17)	0.0068 (18)	0.0092 (19)
C51	0.076 (3)	0.139 (4)	0.060 (2)	−0.020 (2)	0.0110 (19)	−0.025 (2)
C52	0.067 (2)	0.129 (3)	0.074 (2)	−0.034 (2)	0.0202 (19)	−0.022 (2)
C19	0.0418 (17)	0.107 (3)	0.087 (2)	0.0042 (18)	0.0012 (16)	−0.042 (2)
C20	0.053 (3)	0.088 (4)	0.075 (3)	0.023 (3)	0.007 (3)	−0.017 (3)
C21	0.067 (3)	0.057 (3)	0.078 (3)	0.011 (2)	0.007 (2)	−0.014 (2)
C20'	0.039 (7)	0.062 (11)	0.072 (12)	−0.013 (8)	0.009 (7)	−0.025 (8)
C21'	0.070 (10)	0.049 (10)	0.084 (13)	−0.020 (8)	0.017 (9)	−0.026 (9)
O1	0.0574 (13)	0.0573 (12)	0.0470 (11)	−0.0104 (11)	0.0023 (10)	0.0029 (10)
P1	0.0731 (6)	0.0797 (7)	0.0772 (6)	−0.0121 (5)	0.0171 (5)	−0.0017 (5)
F1	0.50 (2)	0.109 (6)	0.129 (8)	−0.002 (9)	0.036 (10)	0.078 (6)
F2	0.066 (3)	0.229 (8)	0.113 (5)	0.017 (3)	0.022 (3)	0.026 (5)
F3	0.142 (5)	0.172 (6)	0.112 (5)	0.048 (4)	−0.023 (4)	0.035 (4)

F4	0.126 (6)	0.201 (9)	0.260 (12)	−0.073 (6)	0.126 (7)	−0.075 (8)
F5	0.166 (7)	0.164 (9)	0.170 (10)	−0.008 (7)	−0.013 (8)	−0.105 (8)
F6	0.201 (7)	0.132 (6)	0.078 (3)	−0.078 (5)	0.006 (4)	−0.017 (3)
F1'	0.41 (3)	0.31 (3)	0.066 (6)	−0.02 (2)	0.019 (11)	−0.035 (11)
F2'	0.070 (6)	0.306 (19)	0.245 (18)	0.048 (8)	−0.029 (8)	0.012 (15)
F3'	0.45 (4)	0.35 (3)	0.120 (10)	−0.03 (3)	0.164 (17)	0.057 (14)
F4'	0.204 (15)	0.210 (14)	0.197 (15)	0.173 (13)	−0.020 (12)	0.011 (10)
F5'	0.211 (14)	0.094 (7)	0.207 (19)	−0.051 (7)	−0.027 (16)	−0.012 (10)
F6'	0.38 (3)	0.183 (18)	0.38 (3)	−0.22 (2)	0.04 (3)	0.05 (2)
P2	0.0945 (8)	0.0867 (7)	0.0619 (6)	−0.0170 (6)	−0.0218 (5)	0.0009 (5)
F7	0.170 (19)	0.16 (2)	0.22 (2)	−0.029 (16)	0.094 (16)	−0.021 (16)
F8	0.198 (19)	0.134 (14)	0.173 (19)	−0.058 (15)	−0.139 (16)	0.036 (14)
F9	0.106 (10)	0.23 (2)	0.18 (2)	−0.065 (9)	0.026 (10)	0.098 (17)
F10	0.173 (19)	0.103 (9)	0.125 (10)	0.010 (8)	−0.086 (12)	0.010 (7)
F11	0.33 (3)	0.20 (2)	0.075 (9)	0.025 (17)	0.082 (15)	−0.052 (10)
F12	0.20 (2)	0.166 (15)	0.24 (2)	−0.014 (12)	0.014 (15)	−0.126 (14)
F7'	0.133 (6)	0.141 (6)	0.101 (4)	0.043 (5)	0.039 (3)	0.058 (4)
F8'	0.141 (6)	0.143 (6)	0.181 (9)	0.052 (5)	−0.091 (5)	−0.024 (5)
F9'	0.328 (16)	0.152 (7)	0.093 (4)	−0.077 (9)	0.009 (7)	0.023 (4)
F10'	0.063 (4)	0.305 (13)	0.190 (9)	−0.018 (5)	−0.003 (4)	0.024 (7)
F11'	0.149 (5)	0.082 (4)	0.134 (7)	−0.023 (3)	−0.021 (4)	−0.024 (3)
F12'	0.192 (8)	0.092 (4)	0.124 (5)	−0.031 (3)	−0.066 (5)	−0.020 (3)

Geometric parameters (Å, °)

Mn1—O2	2.1829 (19)	C33—C34	1.507 (5)
Mn1—O3	2.196 (2)	C33—H33A	0.9700
Mn1—N4	2.267 (2)	C33—H33B	0.9700
Mn1—N2	2.283 (2)	C34—C35	1.505 (4)
Mn1—N1	2.285 (2)	C34—H34A	0.9700
Mn1—N3	2.286 (2)	C34—H34B	0.9700
N1—C5	1.337 (3)	C35—C36	1.380 (4)
N1—C1	1.340 (3)	C35—C38	1.381 (4)
N2—C18	1.337 (3)	C36—C37	1.368 (4)
N2—C14	1.339 (3)	C36—H36A	0.9300
N3—C27	1.337 (4)	C37—H37A	0.9300
N3—C31	1.338 (3)	C38—C39	1.373 (4)
N4—C44	1.333 (3)	C38—H38A	0.9300
N4—C40	1.334 (3)	C39—H39A	0.9300
N5—C11	1.327 (4)	C40—C41	1.373 (4)
N5—C12	1.329 (4)	C40—H40A	0.9300
N6—C24	1.325 (4)	C41—C42	1.379 (4)
N6—C25	1.330 (4)	C41—H41A	0.9300
N7—C39	1.332 (4)	C42—C43	1.381 (4)
N7—C37	1.337 (4)	C42—C45	1.505 (4)
N8—C50	1.321 (4)	C43—C44	1.369 (4)
N8—C51	1.321 (4)	C43—H43A	0.9300
O2—H21	0.85 (4)	C44—H44A	0.9300
O2—H22	0.80 (4)	C45—C46	1.519 (4)

O3—H31	0.79 (4)	C45—H45A	0.9700
O3—H32	0.83 (4)	C45—H45B	0.9700
C1—C2	1.372 (4)	C46—C47	1.499 (4)
C1—H1A	0.9300	C46—H46A	0.9700
C2—C3	1.382 (4)	C46—H46B	0.9700
C2—H2A	0.9300	C47—C48	1.516 (4)
C3—C4	1.390 (4)	C47—H47A	0.9700
C3—C6	1.500 (4)	C47—H47B	0.9700
C4—C5	1.374 (4)	C48—C49	1.359 (4)
C4—H4A	0.9300	C48—C52	1.385 (5)
C5—H5A	0.9300	C49—C50	1.371 (4)
C6—C7	1.533 (4)	C49—H49A	0.9300
C6—H6A	0.9700	C50—H50A	0.9300
C6—H6B	0.9700	C51—C52	1.381 (5)
C7—C8	1.500 (4)	C51—H51A	0.9300
C7—H7A	0.9700	C52—H52A	0.9300
C7—H7B	0.9700	C19—C20'	1.551 (9)
C8—C9	1.512 (4)	C19—C20	1.567 (5)
C8—H8A	0.9700	C19—H19A	0.9700
C8—H8B	0.9700	C19—H19B	0.9700
C9—C13	1.372 (4)	C19—H19C	0.9701
C9—C10	1.378 (4)	C19—H19D	0.9699
C10—C11	1.374 (4)	C20—C21	1.509 (6)
C10—H10A	0.9300	C20—H20A	0.9700
C11—H11A	0.9300	C20—H20B	0.9700
C12—C13	1.375 (4)	C21—H21A	0.9700
C12—H12A	0.9300	C21—H21B	0.9700
C13—H13A	0.9300	C20'—C21'	1.525 (10)
C14—C15	1.379 (4)	C20'—H20C	0.9700
C14—H14A	0.9300	C20'—H20D	0.9700
C15—C16	1.384 (4)	C21'—H21C	0.9700
C15—H15A	0.9300	C21'—H21D	0.9700
C16—C17	1.380 (4)	O1—H11	0.85 (4)
C16—C19	1.509 (4)	O1—H12	0.86 (4)
C17—C18	1.373 (4)	P1—F1	1.501 (6)
C17—H17A	0.9300	P1—F2	1.552 (4)
C18—H18A	0.9300	P1—F3	1.572 (5)
C22—C26	1.377 (4)	P1—F4	1.520 (5)
C22—C23	1.386 (4)	P1—F5	1.512 (6)
C22—C21	1.537 (5)	P1—F6	1.582 (5)
C22—C21'	1.581 (9)	P1—F1'	1.525 (9)
C23—C24	1.372 (4)	P1—F2'	1.562 (8)
C23—H23A	0.9300	P1—F3'	1.494 (8)
C24—H24A	0.9300	P1—F4'	1.500 (7)
C25—C26	1.372 (4)	P1—F5'	1.525 (9)
C25—H25A	0.9300	P1—F6'	1.508 (9)
C26—H26A	0.9300	P2—F7	1.549 (10)
C27—C28	1.373 (4)	P2—F8	1.551 (9)
C27—H27A	0.9300	P2—F9	1.560 (9)

C28—C29	1.375 (4)	P2—F10	1.583 (9)
C28—H28A	0.9300	P2—F11	1.535 (9)
C29—C30	1.373 (5)	P2—F12	1.546 (9)
C29—C32	1.508 (4)	P2—F7'	1.539 (4)
C30—C31	1.381 (4)	P2—F8'	1.534 (6)
C30—H30A	0.9300	P2—F9'	1.555 (6)
C31—H31A	0.9300	P2—F10'	1.547 (6)
C32—C33	1.530 (5)	P2—F11'	1.566 (5)
C32—H32A	0.9700	P2—F12'	1.569 (5)
C32—H32B	0.9700		
O2—Mn1—O3	173.03 (8)	C35—C36—H36A	119.8
O2—Mn1—N4	89.70 (8)	N7—C37—C36	123.8 (3)
O3—Mn1—N4	92.58 (8)	N7—C37—H37A	118.1
O2—Mn1—N2	87.70 (8)	C36—C37—H37A	118.1
O3—Mn1—N2	90.10 (8)	C39—C38—C35	120.1 (3)
N4—Mn1—N2	177.28 (8)	C39—C38—H38A	119.9
O2—Mn1—N1	88.69 (8)	C35—C38—H38A	119.9
O3—Mn1—N1	84.69 (8)	N7—C39—C38	123.8 (3)
N4—Mn1—N1	91.03 (8)	N7—C39—H39A	118.1
N2—Mn1—N1	89.71 (8)	C38—C39—H39A	118.1
O2—Mn1—N3	94.28 (8)	N4—C40—C41	123.2 (3)
O3—Mn1—N3	92.31 (8)	N4—C40—H40A	118.4
N4—Mn1—N3	89.65 (8)	C41—C40—H40A	118.4
N2—Mn1—N3	89.75 (8)	C40—C41—C42	120.5 (3)
N1—Mn1—N3	176.96 (8)	C40—C41—H41A	119.7
C5—N1—C1	116.3 (2)	C42—C41—H41A	119.7
C5—N1—Mn1	121.23 (18)	C41—C42—C43	116.0 (3)
C1—N1—Mn1	121.46 (19)	C41—C42—C45	122.1 (3)
C18—N2—C14	116.2 (2)	C43—C42—C45	121.9 (3)
C18—N2—Mn1	121.17 (19)	C44—C43—C42	120.4 (3)
C14—N2—Mn1	121.64 (18)	C44—C43—H43A	119.8
C27—N3—C31	115.8 (3)	C42—C43—H43A	119.8
C27—N3—Mn1	120.26 (19)	N4—C44—C43	123.5 (3)
C31—N3—Mn1	123.9 (2)	N4—C44—H44A	118.3
C44—N4—C40	116.4 (2)	C43—C44—H44A	118.3
C44—N4—Mn1	121.04 (18)	C42—C45—C46	112.3 (3)
C40—N4—Mn1	122.24 (19)	C42—C45—H45A	109.1
C11—N5—C12	115.6 (3)	C46—C45—H45A	109.1
C24—N6—C25	115.9 (3)	C42—C45—H45B	109.1
C39—N7—C37	115.8 (3)	C46—C45—H45B	109.1
C50—N8—C51	115.5 (3)	H45A—C45—H45B	107.9
Mn1—O2—H21	123 (2)	C47—C46—C45	112.5 (3)
Mn1—O2—H22	129 (3)	C47—C46—H46A	109.1
H21—O2—H22	108 (3)	C45—C46—H46A	109.1
Mn1—O3—H31	125 (3)	C47—C46—H46B	109.1
Mn1—O3—H32	126 (2)	C45—C46—H46B	109.1
H31—O3—H32	108 (3)	H46A—C46—H46B	107.8
N1—C1—C2	123.3 (3)	C46—C47—C48	116.1 (3)
N1—C1—H1A	118.4	C46—C47—H47A	108.3

C2—C1—H1A	118.4	C48—C47—H47A	108.3
C1—C2—C3	120.6 (3)	C46—C47—H47B	108.3
C1—C2—H2A	119.7	C48—C47—H47B	108.3
C3—C2—H2A	119.7	H47A—C47—H47B	107.4
C2—C3—C4	116.1 (3)	C49—C48—C52	115.9 (3)
C2—C3—C6	122.3 (3)	C49—C48—C47	120.0 (3)
C4—C3—C6	121.6 (3)	C52—C48—C47	124.1 (3)
C5—C4—C3	120.0 (3)	C48—C49—C50	120.2 (3)
C5—C4—H4A	120.0	C48—C49—H49A	119.9
C3—C4—H4A	120.0	C50—C49—H49A	119.9
N1—C5—C4	123.6 (3)	N8—C50—C49	124.7 (3)
N1—C5—H5A	118.2	N8—C50—H50A	117.7
C4—C5—H5A	118.2	C49—C50—H50A	117.7
C3—C6—C7	112.8 (2)	N8—C51—C52	123.5 (4)
C3—C6—H6A	109.0	N8—C51—H51A	118.3
C7—C6—H6A	109.0	C52—C51—H51A	118.3
C3—C6—H6B	109.0	C51—C52—C48	120.1 (3)
C7—C6—H6B	109.0	C51—C52—H52A	119.9
H6A—C6—H6B	107.8	C48—C52—H52A	119.9
C8—C7—C6	114.3 (3)	C16—C19—C20'	115.4 (7)
C8—C7—H7A	108.7	C16—C19—C20	110.8 (3)
C6—C7—H7A	108.7	C16—C19—H19A	109.5
C8—C7—H7B	108.7	C20—C19—H19A	109.5
C6—C7—H7B	108.7	C16—C19—H19B	109.5
H7A—C7—H7B	107.6	C20—C19—H19B	109.5
C7—C8—C9	115.3 (3)	H19A—C19—H19B	108.1
C7—C8—H8A	108.5	C16—C19—H19C	108.3
C9—C8—H8A	108.5	C20'—C19—H19C	108.3
C7—C8—H8B	108.5	C16—C19—H19D	109.0
C9—C8—H8B	108.5	C20'—C19—H19D	107.9
H8A—C8—H8B	107.5	H19C—C19—H19D	107.8
C13—C9—C10	116.1 (3)	C21—C20—C19	111.6 (4)
C13—C9—C8	122.4 (3)	C21—C20—H20A	109.3
C10—C9—C8	121.4 (3)	C19—C20—H20A	109.3
C11—C10—C9	119.9 (3)	C21—C20—H20B	109.3
C11—C10—H10A	120.0	C19—C20—H20B	109.3
C9—C10—H10A	120.0	H20A—C20—H20B	108.0
N5—C11—C10	124.2 (3)	C20—C21—C22	109.8 (4)
N5—C11—H11A	117.9	C20—C21—H21A	109.7
C10—C11—H11A	117.9	C22—C21—H21A	109.7
N5—C12—C13	123.8 (3)	C20—C21—H21B	109.7
N5—C12—H12A	118.1	C22—C21—H21B	109.7
C13—C12—H12A	118.1	H21A—C21—H21B	108.2
C9—C13—C12	120.4 (3)	C21'—C20'—C19	112.5 (8)
C9—C13—H13A	119.8	C21'—C20'—H20C	109.1
C12—C13—H13A	119.8	C19—C20'—H20C	109.1
N2—C14—C15	123.5 (3)	C21'—C20'—H20D	109.1
N2—C14—H14A	118.3	C19—C20'—H20D	109.1
C15—C14—H14A	118.3	H20C—C20'—H20D	107.8

C14—C15—C16	119.9 (3)	C20'—C21'—C22	105.9 (8)
C14—C15—H15A	120.1	C20'—C21'—H21C	110.6
C16—C15—H15A	120.1	C22—C21'—H21C	110.6
C17—C16—C15	116.6 (3)	C20'—C21'—H21D	110.6
C17—C16—C19	122.0 (3)	C22—C21'—H21D	110.6
C15—C16—C19	121.4 (3)	H21C—C21'—H21D	108.7
C18—C17—C16	120.2 (3)	H11—O1—H12	114 (3)
C18—C17—H17A	119.9	F1—P1—F5	97.0 (6)
C16—C17—H17A	119.9	F1—P1—F4	88.5 (8)
N2—C18—C17	123.6 (3)	F5—P1—F4	92.8 (6)
N2—C18—H18A	118.2	F1—P1—F2	92.3 (7)
C17—C18—H18A	118.2	F5—P1—F2	93.0 (6)
C26—C22—C23	116.3 (3)	F4—P1—F2	174.0 (5)
C26—C22—C21	122.6 (3)	F1—P1—F3	172.9 (6)
C23—C22—C21	120.6 (3)	F5—P1—F3	90.0 (6)
C26—C22—C21'	114.1 (5)	F4—P1—F3	92.5 (5)
C23—C22—C21'	118.2 (7)	F2—P1—F3	85.9 (4)
C24—C23—C22	119.5 (3)	F1—P1—F6	86.3 (5)
C24—C23—H23A	120.3	F5—P1—F6	176.4 (7)
C22—C23—H23A	120.3	F4—P1—F6	85.9 (5)
N6—C24—C23	124.4 (3)	F2—P1—F6	88.3 (4)
N6—C24—H24A	117.8	F3—P1—F6	86.8 (4)
C23—C24—H24A	117.8	F3'—P1—F4'	98.8 (13)
N6—C25—C26	123.7 (3)	F3'—P1—F6'	95.8 (13)
N6—C25—H25A	118.1	F4'—P1—F6'	97.1 (14)
C26—C25—H25A	118.1	F3'—P1—F1'	169.0 (15)
C25—C26—C22	120.2 (3)	F4'—P1—F1'	90.5 (12)
C25—C26—H26A	119.9	F6'—P1—F1'	88.8 (11)
C22—C26—H26A	119.9	F3'—P1—F5'	88.8 (10)
N3—C27—C28	123.6 (3)	F4'—P1—F5'	92.3 (13)
N3—C27—H27A	118.2	F6'—P1—F5'	168.7 (15)
C28—C27—H27A	118.2	F1'—P1—F5'	85.0 (11)
C27—C28—C29	120.5 (3)	F3'—P1—F2'	89.7 (12)
C27—C28—H28A	119.7	F4'—P1—F2'	165.7 (10)
C29—C28—H28A	119.7	F6'—P1—F2'	93.4 (14)
C30—C29—C28	116.4 (3)	F1'—P1—F2'	80.1 (12)
C30—C29—C32	123.0 (3)	F5'—P1—F2'	76.3 (12)
C28—C29—C32	120.6 (3)	F11—P2—F12	173.8 (15)
C29—C30—C31	120.3 (3)	F11—P2—F7	100.3 (17)
C29—C30—H30A	119.9	F12—P2—F7	79.4 (19)
C31—C30—H30A	119.9	F11—P2—F8	85.8 (15)
N3—C31—C30	123.5 (3)	F12—P2—F8	88.0 (14)
N3—C31—H31A	118.3	F7—P2—F8	90.8 (17)
C30—C31—H31A	118.3	F7—P2—F9	172.7 (17)
C29—C32—C33	112.6 (3)	F8—P2—F9	94.2 (15)
C29—C32—H32A	109.1	F11—P2—F9	85.3 (16)
C33—C32—H32A	109.1	F11—P2—F10	83.0 (14)
C29—C32—H32B	109.1	F12—P2—F10	103.2 (14)
C33—C32—H32B	109.1	F7—P2—F10	87.8 (14)

H32A—C32—H32B	107.8	F8—P2—F10	168.3 (13)
C34—C33—C32	113.7 (3)	F9—P2—F10	88.4 (12)
C34—C33—H33A	108.8	F12—P2—F9	95.4 (17)
C32—C33—H33A	108.8	F8'—P2—F7'	91.5 (7)
C34—C33—H33B	108.8	F8'—P2—F10'	176.2 (7)
C32—C33—H33B	108.8	F7'—P2—F10'	89.8 (6)
H33A—C33—H33B	107.7	F8'—P2—F9'	88.3 (8)
C35—C34—C33	112.5 (3)	F7'—P2—F9'	176.9 (7)
C35—C34—H34A	109.1	F10'—P2—F9'	90.7 (7)
C33—C34—H34A	109.1	F8'—P2—F11'	92.0 (6)
C35—C34—H34B	109.1	F7'—P2—F11'	85.3 (7)
C33—C34—H34B	109.1	F10'—P2—F11'	91.6 (6)
H34A—C34—H34B	107.8	F9'—P2—F11'	91.7 (6)
C36—C35—C38	116.1 (3)	F8'—P2—F12'	90.2 (6)
C36—C35—C34	122.4 (3)	F7'—P2—F12'	92.7 (7)
C38—C35—C34	121.4 (3)	F10'—P2—F12'	86.3 (6)
C37—C36—C35	120.3 (3)	F9'—P2—F12'	90.4 (6)
C37—C36—H36A	119.8	F11'—P2—F12'	177.1 (5)
O2—Mn1—N1—C5	−141.1 (2)	C22—C23—C24—N6	1.0 (5)
O3—Mn1—N1—C5	41.0 (2)	C24—N6—C25—C26	−0.2 (5)
N4—Mn1—N1—C5	−51.4 (2)	N6—C25—C26—C22	−0.1 (5)
N2—Mn1—N1—C5	131.2 (2)	C23—C22—C26—C25	0.8 (5)
O2—Mn1—N1—C1	50.6 (2)	C21—C22—C26—C25	−170.8 (4)
O3—Mn1—N1—C1	−127.2 (2)	C21'—C22—C26—C25	143.7 (7)
N4—Mn1—N1—C1	140.3 (2)	C31—N3—C27—C28	−0.6 (4)
N2—Mn1—N1—C1	−37.1 (2)	Mn1—N3—C27—C28	178.5 (2)
O2—Mn1—N2—C18	−128.8 (2)	N3—C27—C28—C29	0.6 (5)
O3—Mn1—N2—C18	44.6 (2)	C27—C28—C29—C30	0.1 (5)
N1—Mn1—N2—C18	−40.1 (2)	C27—C28—C29—C32	−179.0 (3)
N3—Mn1—N2—C18	136.9 (2)	C28—C29—C30—C31	−0.7 (5)
O2—Mn1—N2—C14	39.2 (2)	C32—C29—C30—C31	178.4 (3)
O3—Mn1—N2—C14	−147.4 (2)	C27—N3—C31—C30	−0.1 (4)
N1—Mn1—N2—C14	127.9 (2)	Mn1—N3—C31—C30	−179.1 (2)
N3—Mn1—N2—C14	−55.1 (2)	C29—C30—C31—N3	0.7 (5)
O2—Mn1—N3—C27	−130.5 (2)	C30—C29—C32—C33	−108.8 (4)
O3—Mn1—N3—C27	47.2 (2)	C28—C29—C32—C33	70.3 (4)
N4—Mn1—N3—C27	139.8 (2)	C29—C32—C33—C34	68.0 (4)
N2—Mn1—N3—C27	−42.9 (2)	C32—C33—C34—C35	−176.0 (3)
O2—Mn1—N3—C31	48.4 (2)	C33—C34—C35—C36	112.1 (4)
O3—Mn1—N3—C31	−133.8 (2)	C33—C34—C35—C38	−67.1 (4)
N4—Mn1—N3—C31	−41.3 (2)	C38—C35—C36—C37	−0.2 (5)
N2—Mn1—N3—C31	136.1 (2)	C34—C35—C36—C37	−179.4 (3)
O2—Mn1—N4—C44	37.3 (2)	C39—N7—C37—C36	−1.2 (5)
O3—Mn1—N4—C44	−136.1 (2)	C35—C36—C37—N7	0.9 (5)
N1—Mn1—N4—C44	−51.4 (2)	C36—C35—C38—C39	0.0 (5)
N3—Mn1—N4—C44	131.6 (2)	C34—C35—C38—C39	179.2 (3)
O2—Mn1—N4—C40	−135.7 (2)	C37—N7—C39—C38	1.0 (5)
O3—Mn1—N4—C40	50.9 (2)	C35—C38—C39—N7	−0.4 (5)
N1—Mn1—N4—C40	135.6 (2)	C44—N4—C40—C41	−2.0 (5)

N3—Mn1—N4—C40	−41.4 (2)	Mn1—N4—C40—C41	171.3 (3)
C5—N1—C1—C2	−2.3 (4)	N4—C40—C41—C42	1.0 (5)
Mn1—N1—C1—C2	166.5 (2)	C40—C41—C42—C43	1.0 (5)
N1—C1—C2—C3	−0.3 (4)	C40—C41—C42—C45	−178.1 (3)
C1—C2—C3—C4	2.6 (4)	C41—C42—C43—C44	−1.9 (4)
C1—C2—C3—C6	−175.4 (3)	C45—C42—C43—C44	177.2 (3)
C2—C3—C4—C5	−2.3 (4)	C40—N4—C44—C43	1.1 (4)
C6—C3—C4—C5	175.6 (3)	Mn1—N4—C44—C43	−172.3 (2)
C1—N1—C5—C4	2.5 (4)	C42—C43—C44—N4	0.9 (5)
Mn1—N1—C5—C4	−166.3 (2)	C41—C42—C45—C46	62.0 (4)
C3—C4—C5—N1	−0.2 (4)	C43—C42—C45—C46	−117.0 (3)
C2—C3—C6—C7	88.4 (4)	C42—C45—C46—C47	179.5 (3)
C4—C3—C6—C7	−89.4 (4)	C45—C46—C47—C48	−176.6 (3)
C3—C6—C7—C8	−64.9 (4)	C46—C47—C48—C49	156.7 (3)
C6—C7—C8—C9	−173.0 (3)	C46—C47—C48—C52	−22.8 (5)
C7—C8—C9—C13	−132.7 (3)	C52—C48—C49—C50	−3.0 (5)
C7—C8—C9—C10	48.8 (5)	C47—C48—C49—C50	177.5 (3)
C13—C9—C10—C11	−1.4 (5)	C51—N8—C50—C49	1.7 (5)
C8—C9—C10—C11	177.2 (3)	C48—C49—C50—N8	1.5 (5)
C12—N5—C11—C10	−0.1 (5)	C50—N8—C51—C52	−3.3 (6)
C9—C10—C11—N5	1.2 (6)	N8—C51—C52—C48	1.7 (7)
C11—N5—C12—C13	−0.7 (5)	C49—C48—C52—C51	1.5 (6)
C10—C9—C13—C12	0.7 (5)	C47—C48—C52—C51	−179.0 (4)
C8—C9—C13—C12	−177.9 (3)	C17—C16—C19—C20'	57.6 (8)
N5—C12—C13—C9	0.4 (6)	C15—C16—C19—C20'	−120.5 (7)
C18—N2—C14—C15	2.0 (4)	C17—C16—C19—C20	93.5 (4)
Mn1—N2—C14—C15	−166.6 (2)	C15—C16—C19—C20	−84.6 (4)
N2—C14—C15—C16	0.3 (5)	C16—C19—C20—C21	−68.0 (6)
C14—C15—C16—C17	−2.6 (4)	C20'—C19—C20—C21	36.9 (11)
C14—C15—C16—C19	175.6 (3)	C19—C20—C21—C22	−174.6 (3)
C15—C16—C17—C18	2.7 (4)	C26—C22—C21—C20	−119.1 (5)
C19—C16—C17—C18	−175.5 (3)	C23—C22—C21—C20	69.8 (6)
C14—N2—C18—C17	−1.9 (4)	C21'—C22—C21—C20	−29.1 (8)
Mn1—N2—C18—C17	166.7 (2)	C16—C19—C20'—C21'	62.6 (16)
C16—C17—C18—N2	−0.5 (5)	C20—C19—C20'—C21'	−27.0 (9)
C26—C22—C23—C24	−1.2 (5)	C19—C20'—C21'—C22	−173.7 (10)
C21—C22—C23—C24	170.5 (4)	C26—C22—C21'—C20'	148.5 (11)
C21'—C22—C23—C24	−142.5 (6)	C23—C22—C21'—C20'	−69.4 (14)
C25—N6—C24—C23	−0.3 (5)	C21—C22—C21'—C20'	35.8 (9)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H21···O1	0.85 (4)	1.85 (4)	2.693 (3)	173 (3)
O1—H11···N7^{i}	0.85 (4)	1.94 (4)	2.775 (3)	169 (3)
O1—H12···N8^{ii}	0.86 (4)	1.90 (4)	2.752 (3)	172 (3)
O2—H22···N5^{iii}	0.80 (4)	2.02 (4)	2.818 (3)	174 (4)
O3—H31···N6^{iv}	0.79 (4)	2.07 (4)	2.861 (3)	174 (4)

O3—H32···O1^{v}	0.83 (4)	1.92 (4)	2.733 (3)	169 (3)

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*; (ii) *x*−1/2, −*y*+1/2, −*z*; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) −*x*+1, *y*−1/2, −*z*+1/2; (v) −*x*+3/2, *y*−1/2, *z*.

Fig. 1